

Spin-dependent Hedin's equations

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Hedin's equations for the electron self-energy and the vertex were originally derived for a many-electron system with Coulomb interaction. In recent years it has been increasingly recognized that spin interactions can play a major role in determining physical properties of systems such as nanoscale magnets or of interfaces and surfaces. We derive a generalized set of Hedin's equations for quantum many-body systems containing spin interactions, e.g. spin-orbit and spin-spin interactions. The corresponding spin-dependent GW approximation is constructed.

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An increasing number of modern applications of materials science imply spin degrees of freedom. Spintronics devices, colossal magneto resistance materials or magnetic impurities in semiconductors are important examples, not only due to their technological interest but also owing to the fundamental questions they raise. In fact, a detailed understanding of such systems requires a theoretical description of the interplay of spin, charge and orbital degrees of freedom, and relies crucially on a reliable description of electronic interactions. In striking contrast to these scientific and technological needs, the actual progress in developing techniques for describing interaction effects beyond density functional theory [1] in an explicitly spin-dependent manner has been slow. In particular, one of the most important first principles many-body methods used nowadays for describing electronic excitations, the so-called GW method, still awaits its extension to spin-dependent interactions.

In 1965, Hedin derived a closed set of equations for the electronic Green's function and self-energy, the screened Coulomb interaction and the polarization of a solid [2]. The equations provide an iterative scheme for an expansion of the self-energy in powers of the screened interaction. Although there is no guarantee that the iterative procedure is absolutely convergent, as originally envisioned by Hedin, it nevertheless provides a rigorous basis for studying the self-energy of real materials from first-principles. In particular, the lowest order approximation leads to the *GW* approximation (GWA) [2, 3, 4] which has proven very successful in studying one-particle excitation energies of real materials entirely from first-principles.

The original Hedin's equations were derived for a many-body Hamiltonian with a Coulomb interaction only, without the possibility of having an explicit spin-dependent interaction. The GWA derived from them has met tremendous progress in describing the electronic structure and excitation spectra of semiconductor-based systems, transition metals and oxides. Due to their restriction to spin-independent interactions it has however not been useful for studying correlation effects arising

from spin-dependent interactions in the classes of materials mentioned above. These interactions are crucial, despite the tiny energy scales associated with them. To cite an example, the conduction band spin splitting in zinc blende semiconductors arising from spin-orbit coupling is only tens of *meV* and yet it is important for applications in spintronics since it determines the spin lifetimes as well as inducing spin current in the absence of a magnetic field, the so-called Rashba effect [5].

The aim of the present work is to present generalized Hedin's equations, suitable for dealing with explicitly spin-dependent interactions. These interactions may arise from relativistic effects, such as spin-orbit coupling, or from an external perturbation like in the case of a magnetic impurity in a semiconductor. With a spin-dependent interaction it is possible to relate the two-particle Green's function to functional derivatives of the one-particle Green's function with respect to an electric and a magnetic field. The first order term in the screened interaction of the resulting spin-dependent Hedin's equations yields a generalization of the GW approximation.

The Hamiltonian with a spin-dependent two-particle interaction is given by

$$\hat{H}_0 = \sum_{\kappa} \int d^3r \hat{\psi}_{\kappa}^{\dagger}(\mathbf{r}) h_0(\mathbf{r}) \hat{\psi}_{\kappa}(\mathbf{r}) + \frac{1}{2} \sum_{\kappa\beta\gamma\eta} \int d^3r d^3r' \hat{\psi}_{\kappa}^{\dagger}(\mathbf{r}) \hat{\psi}_{\beta}^{\dagger}(\mathbf{r}') v_{\kappa\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') \hat{\psi}_{\eta}(\mathbf{r}') \hat{\psi}_{\gamma}(\mathbf{r}). \quad (1)$$

where h_0 is the one-particle Hamiltonian. The identity of the particles implies that the second term is invariant under particle interchange: $v_{\kappa\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') \leftrightarrow v_{\beta\eta\kappa\gamma}(\mathbf{r}', \mathbf{r})$ [6]. For this general Hamiltonian, we will derive the following set of generalized Hedin's equations, relating the electronic self-energy Σ to the Green's function G and the screened interaction W , using the polarization P and the vertex function Λ :

$$\Sigma_{\alpha\beta}(1, 2) = -\sigma_{\alpha\eta}^I \mathcal{G}_{\eta\gamma}(1, 4) \Lambda_{\gamma\beta}^J(4, 2, 5) W_{JI}(5, 1), \quad (2)$$

$$W_{IJ}(1, 2) = v_{IJ}(1, 2) + v_{IK}(1, 3)P_{KL}(3, 4)W_{LJ}(4, 2), \quad (3)$$

$$P_{IJ}(1, 2) = \sigma_{\alpha\beta}^I \mathcal{G}_{\beta\gamma}(1, 3) \Lambda_{\gamma\eta}^J(3, 4, 2) \mathcal{G}_{\eta\alpha}(4, 1^+), \quad (4)$$

$$\Lambda_{\alpha\beta}^I(1, 2, 3) = \delta(1-2)\delta(2-3)\sigma_{\alpha\beta}^I + \frac{\delta\Sigma_{\alpha\beta}(1, 2)}{\delta\mathcal{G}_{\gamma\eta}(4, 5)} \mathcal{G}_{\eta\eta'}(4, 6) \Lambda_{\eta'\kappa}^I(6, 7, 3) \mathcal{G}_{\kappa\gamma}(7, 5). \quad (5)$$

Here, σ^i , $i=x,y,z$, are the Pauli spin matrices and σ^0 is defined to be a 2x2 unit matrix. Capital letter indices run over 0,x,y,z, while Greek letters take the values ± 1 . We use the following common shorthand notation: $(\mathbf{x}\tau)$ is represented by a number, repeated indices are summed and repeated variables represented by numbers are integrated, unless they appear on both sides of the equation. For clarity, we further adopt a notation that quantities with subscript denoted by capital letter do not depend on spin. The spin-dependent interaction has been expanded in the Pauli and unit matrices as

$$v_{\alpha\eta\kappa\gamma}(1, 2) = \sigma_{\alpha\eta}^I v_{IJ}(1, 2) \sigma_{\kappa\gamma}^J. \quad (6)$$

The spin-Hedin equations can e.g. be applied to Hamiltonians containing interactions of the following form.

$$v_{\alpha\gamma\beta\eta}(\mathbf{r}, \mathbf{r}') = \begin{cases} \sigma_{\alpha\gamma}^0 \sigma_{\beta\eta}^0 / |\mathbf{r} - \mathbf{r}'|, \\ \sigma_{\alpha\gamma}^i J_{ij}(\mathbf{r}, \mathbf{r}') \sigma_{\beta\eta}^j, \\ \sigma_{\alpha\gamma}^i \mu_i(\mathbf{r}, \mathbf{r}') \sigma_{\beta\eta}^0 \end{cases} \quad (7)$$

where the first is the usual Coulomb interaction, the second a spin-spin interaction and the third a spin-orbit interaction, which contains the angular momentum operator.

The general structure of the set of equations (2) – (5) is remarkably close to the usual Hedin's equations. However, the self-energy now depends on the spin variable, and the screened interaction W as well as the polarization function P acquire a matrix form expressing an interplay between the charge and spin channels. Thus, a polarization function P_{0i} , for example, describes a charge density response of the system with respect to a perturbing magnetic field in the i -direction. When P is used in (3) the charge channel of the screened interaction experiences the effects of the spin interactions and vice versa.

Most importantly, one can construct from these equations a spin-dependent generalization of Hedin's GWA, by approximating the vertex functions by

$$\Lambda_{\alpha\beta}^I(1, 2, 3) = \delta(1-2)\delta(2-3)\sigma_{\alpha\beta}^I. \quad (8)$$

The polarization then becomes

$$P_{IJ}(1, 2) = \sigma_{\alpha\beta}^I \mathcal{G}_{\beta\gamma}(1, 2) \sigma_{\gamma\eta}^J \mathcal{G}_{\eta\alpha}(2, 1^+) \quad (9)$$

yielding the self-energy

$$\Sigma_{\alpha\beta}^{GW}(1, 2) = -\sigma_{\alpha\eta}^I \mathcal{G}_{\eta\gamma}(1, 2) \sigma_{\gamma\beta}^J W_{JI}(2, 1). \quad (10)$$

Before proceeding further, let us interpret the meaning of the resulting polarization and the spin-dependent self-energy. Consider first the case $I = J = 0$ (charge channel) giving $P_{00}(1, 2) = \mathcal{G}_{\alpha\gamma}(1, 2) \mathcal{G}_{\gamma\alpha}(2, 1^+)$ and $\Sigma_{\alpha\beta}(1, 2) = -\mathcal{G}_{\alpha\beta}(1, 2) W_{00}(2, 1)$. If the Green function is diagonal in spin space we recover the polarization and the self-energy in the original Hedin's equations. However, for a system with an existing spin structure, such as a non-collinear spin, the Green function possesses non-diagonal spin components. This case is a generalization of the original Hedin's equations to spin-dependent Green's function and self-energy with purely Coulombic interaction. It emerges naturally in the present formulation as a special case where spin interactions are absent.

Let us now consider the case when the interaction is spin dependent, which may arise from purely spin-spin interaction or spin-orbit coupling, among other possibilities. The exchange-correlation effects on the Green function of up spin is illustrated in Fig. 1 (lower panel). A particle of up spin $\mathcal{G}_{\uparrow\uparrow}^0$ enters the self-energy $\Sigma_{\uparrow\uparrow}$. Upon entering the self-energy the electron spin is flipped to down spin by a spin operator $\sigma_{\uparrow\downarrow}^i$ and a magnon represented by W_{ij} is emitted. Upon leaving the self-energy the spin operator $\sigma_{\downarrow\uparrow}^j$ causes the electron to reabsorb the magnon and return to its original up spin configuration. This process is analogous to the original Hedin's GWA whereby an electron emits and absorbs a plasmon but without the possibility of spin flip (upper panel).

The derivation of the generalized Hedin's equations closely follows Hedin's original work, using Schwinger's functional derivative technique. Since many problems related to spin degrees of freedom involves temperature, we work in the finite-temperature formalism but of course the zero-temperature version readily follows. Using the Heisenberg equations of motion we obtain

$$\begin{aligned} & \left[\frac{\partial}{\partial \tau} + h_0(\mathbf{x}) - \mu \right] \mathcal{G}_{\alpha\beta}(\mathbf{x}\tau, \mathbf{x}'\tau') \\ & + \int d^3r v_{\kappa\gamma\alpha\eta}(\mathbf{r}, \mathbf{x}) \mathcal{G}_{\eta\beta\gamma\kappa}^{(2)}(\mathbf{x}\tau, \mathbf{x}'\tau', \mathbf{r}\tau, \mathbf{r}\tau^+) \\ & = -\delta_{\alpha\beta} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \end{aligned} \quad (11)$$

To utilize the Schwinger functional derivative technique we work in the Dirac or interacting representation and define the Green functions as follows.

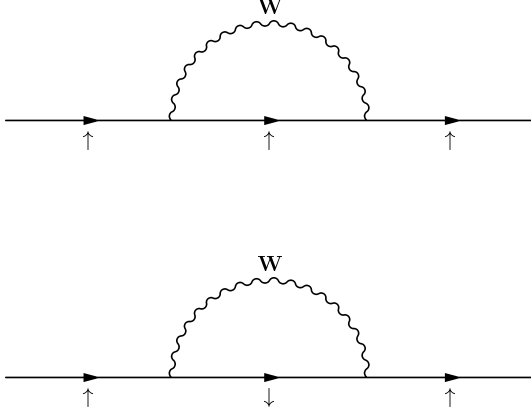


FIG. 1: Diagrams for the self-energy within the spin-dependent GWA, compared with the conventional GWA see text

$$\mathcal{G}_{\alpha\beta}(1, 2) = -\frac{\langle \mathcal{T} [\hat{\mathcal{S}} \hat{\psi}_{\alpha}(1) \hat{\psi}_{\beta}^{\dagger}(2)] \rangle}{\langle \hat{\mathcal{S}} \rangle} \quad (12)$$

$$\mathcal{G}_{\alpha\beta\eta\gamma}^{(2)}(1, 2, 3, 4) = \frac{\langle \mathcal{T} [\hat{\mathcal{S}} \hat{\psi}_{\alpha}(1) \hat{\psi}_{\eta}(3) \hat{\psi}_{\gamma}^{\dagger}(4) \hat{\psi}_{\beta}^{\dagger}(2)] \rangle}{\langle \hat{\mathcal{S}} \rangle} \quad (13)$$

where \mathcal{T} is the imaginary-time-ordering operator and

$$\hat{\mathcal{S}} = \mathcal{T} \exp \left[-\int_0^{\beta} d\tau \hat{\phi}(\tau) \right]. \quad (14)$$

In the original Hedin's derivation a probing electric field was applied to obtain an equation relating the two-particle Green's function to the functional derivative of the one-particle Green's function with respect to the applied electric field. Since we have spin-dependent interactions we have to consider not only a probing electric field, $\varphi_0(\mathbf{r}\tau)$, but also a probing magnetic field, $\varphi_i(\mathbf{r}\tau)$, $i = x, y, z$. The electric and magnetic fields are given by

$$\hat{\phi}(\tau) = \int d^3r \varphi_I(\mathbf{r}\tau) \hat{\psi}_{\alpha}^{\dagger}(\mathbf{r}\tau) \sigma_{\alpha\beta}^I \hat{\psi}_{\beta}(\mathbf{r}\tau). \quad (15)$$

Noting that $\delta\hat{\mathcal{S}}/\delta\varphi_I(1) = -\mathcal{T}[\hat{\mathcal{S}}\hat{\sigma}^I(1)]$ it can be shown

that [7]

$$\frac{\delta\mathcal{G}_{\eta\beta}(1, 2)}{\delta\varphi_I(3)} \quad (16)$$

$$= \left[\mathcal{G}_{\eta\beta}(1, 2) \mathcal{G}_{\gamma\kappa}(3, 3^+) - \mathcal{G}_{\eta\beta\gamma\kappa}^{(2)}(1, 2, 3, 3^+) \right] \sigma_{\kappa\gamma}^I \quad (17)$$

This important relation allows us to replace the two-particle Green's function by a functional derivative of the one-particle Green's function with respect to the applied electric and magnetic field. Using the above relation we define the mass operator \mathcal{M} as follows.

$$\begin{aligned} & \mathcal{M}_{\alpha\gamma}(1, 3) \mathcal{G}_{\gamma\beta}(3, 2) \\ &= v_{\kappa\gamma\alpha\eta}(3, 1) \mathcal{G}_{\eta\beta\gamma\kappa}^{(2)}(1, 2, 3, 3^+) \\ &= v_{IJ}(3, 1) \sigma_{\alpha\eta}^J \left[\mathcal{G}_{\eta\beta}(1, 2) \rho_I(3) - \frac{\delta\mathcal{G}_{\eta\beta}(1, 2)}{\delta\varphi_I(3)} \right]. \end{aligned} \quad (18)$$

The charge and spin density is given by

$$\rho_I(1) = \mathcal{G}_{\gamma\kappa}(1, 1^+) \sigma_{\kappa\gamma}^I. \quad (19)$$

Using the identity

$$(\delta\mathcal{G}/\delta\varphi) = -\mathcal{G}(\delta\mathcal{G}^{-1}/\delta\varphi)\mathcal{G}, \quad (20)$$

multiplying by \mathcal{G}^{-1} on the right and taking out the Hartree-like term (the first term) we obtain from (18) an exact expression for the self-energy:

$$\Sigma_{\alpha\beta}(1, 2) = v_{IJ}(3, 1) \sigma_{\alpha\gamma}^J \mathcal{G}_{\gamma\eta}(1, 4) \frac{\delta\mathcal{G}_{\eta\beta}^{-1}(4, 2)}{\delta\varphi_I(3)}. \quad (21)$$

As pointed out in [7] in the absence of an explicit two-particle spin interaction, only $I = J = 0$ components survive and the self-energy depends only on variation with respect to the electric field φ_0 . Application of a magnetic field introduces a one-particle term in the Hamiltonian but it does not affect the self-energy.

Next, we identify the generalized Hartree potential

$$V_I^H(1) = v_{IJ}(1, 3) \rho_J(3) \quad (22)$$

and the total field $\Phi_I = \varphi_I + V_I^H$. The vertices can then be defined as follows:

$$\Lambda_{\alpha\beta}^I(1, 2, 3) = -\frac{\delta\mathcal{G}_{\alpha\beta}^{-1}(1, 2)}{\delta\Phi_I(3)}. \quad (23)$$

As usual, the dielectric function is related to the derivative of the total field with respect to the applied one

$$\frac{\delta\Phi_I(1)}{\delta\varphi_J(2)} = \varepsilon_{IJ}^{-1}(1, 2) = \delta(1-2)\delta_{IJ} + \frac{\delta V_I^H(1)}{\delta\varphi_J(2)}, \quad (24)$$

Thus, using the chain rule

$$-\frac{\delta \mathcal{G}_{\alpha\beta}^{-1}(1,2)}{\delta \varphi_I(3)} = \Lambda_{\alpha\beta}^J(1,2,4)\varepsilon_{JI}^{-1}(4,3), \quad (25)$$

and inserting this equation into (21) we obtain Eq. (2) with $W_{IJ}(1,2) = \varepsilon_{IK}^{-1}(1,3)v_{KJ}(3,2)$. The charge and spin vertex equations are given by

$$\begin{aligned} \Lambda_{\alpha\beta}^I(1,2,3) &= \delta(1-2)\delta(2-3)\sigma_{\alpha\beta}^I + \frac{\delta \Sigma_{\alpha\beta}(1,2)}{\delta \Phi_I(3)} \\ &= \delta(1-2)\delta(2-3)\sigma_{\alpha\beta}^I \\ &+ \frac{\delta \Sigma_{\alpha\beta}(1,2)}{\delta \mathcal{G}_{\gamma\eta}(4,5)}\mathcal{G}_{\eta\eta'}(4,6)\Lambda_{\eta'\kappa}^I(6,7,3)\mathcal{G}_{\kappa\gamma}(7,5), \end{aligned} \quad (26)$$

where we have made use of the chain rule, the identity (20), and the definition of the vertex in (23).

We now establish the equation for the screened interaction. The polarization is given by the variation of the density with respect to the total field. Using (19), (20), and (23)

$$\begin{aligned} P_{IJ}(1,2) &= \frac{\delta \rho_I(1)}{\delta \Phi_J(2)} \\ &= \sigma_{\alpha\beta}^I \frac{\delta \mathcal{G}_{\beta\alpha}(1,1^+)}{\delta \Phi_J(2)} \\ &= -\sigma_{\alpha\beta}^I \mathcal{G}_{\beta\gamma}(1,3) \frac{\delta \mathcal{G}_{\gamma\eta}^{-1}(3,4)}{\delta \Phi_J(2)} \mathcal{G}_{\eta\alpha}(4,1^+) \\ &= \sigma_{\alpha\beta}^I \mathcal{G}_{\beta\gamma}(1,3) \Lambda_{\gamma\eta}^J(3,4,2) \mathcal{G}_{\eta\alpha}(4,1^+). \end{aligned} \quad (27)$$

Expressing the dielectric function (24) as

$$\begin{aligned} \varepsilon_{IJ}^{-1}(1,2) &= \delta(1-2)\delta_{IJ} + \frac{\delta V_I^H(1)}{\delta \rho_M(3)} \frac{\delta \rho_M(3)}{\delta \Phi_K(4)} \frac{\delta \Phi_K(4)}{\delta \varphi_J(2)} \\ &= \delta(1-2)\delta_{IJ} + v_{IM}(1,3)P_{MK}(3,4)\varepsilon_{KJ}^{-1}(4,2) \end{aligned} \quad (28)$$

and multiplying by the bare interaction, we obtain Eq. (3). The response function, $R = \delta\rho/\delta\varphi$, satisfies a similar equation:

$$R_{IJ}(1,2) = P_{IJ}(1,2) + P_{IK}(1,3)v_{KL}(3,4)R_{KJ}(4,2) \quad (29)$$

which follows from $\delta\rho/\delta\varphi = \delta\rho/\delta\Phi \times \delta\Phi/\delta\varphi = P\varepsilon^{-1}$. The above three equations for ε^{-1} , W , and R are equivalent. This concludes our derivation of the spin-dependent Hedin's equations.

In the following we first comment on some practical aspects of the generalized GWA; we then conclude by discussing possible applications and further developments.

We note that while the magnetic Hedin's equations are exact, the solution depends crucially on the starting

Green's function, when an iterative scheme is used. For example, if we consider an Ising interaction and choose a starting Green's function corresponding to the mean-field solution, solving the magnetic Hedin's equations iteratively will not generate other spin configurations because there is no spin-flip term in the Ising model. More explicitly, the polarization in (9) with the mean-field Green's function will only possess the z-component P_{zz} , which in turns will only generate W_{zz} . Thus, the self-energy in (10) will not have off-diagonal components in spin space that would allow for spin-flip processes yielding spin configurations other than the mean-field one. To solve this problem, one must start with a starting Green's function that corresponds to a multi configuration. This problem does not arise in the general spin spiral case, where the spin at each point may have different magnitude and direction. The non-interacting Green's function [8]

$$\mathcal{G}_{\alpha\beta}^0(\mathbf{r},\mathbf{r}';i\omega) = \sum_n \frac{\phi_{n\alpha}^*(\mathbf{r})\phi_{n\beta}(\mathbf{r}')}{i\omega - \varepsilon_n} \quad (30)$$

possesses non-diagonal components in the spin space which contribute to the charge channel of the polarization.

$$\begin{aligned} P_{00}(1,2) &= \sigma_{\alpha\beta}^0 \mathcal{G}_{\beta\gamma}(1,2) \sigma_{\gamma\eta}^0 \mathcal{G}_{\eta\alpha}(2,1^+) \\ &= \mathcal{G}_{\alpha\gamma}(1,2) \mathcal{G}_{\gamma\alpha}(2,1^+) \end{aligned} \quad (31)$$

and the self-energy naturally acquires non-diagonal components in the spin space.

$$\Sigma_{\alpha\beta}^{GW}(1,2) = -\mathcal{G}_{\alpha\beta}(1,2)W_{00}(2,1). \quad (32)$$

Using the self-energy one solves the quasiparticle equation

$$\begin{pmatrix} h^0 + \Sigma_{\uparrow\uparrow}^{GW}(E_n) & \Sigma_{\uparrow\downarrow}^{GW}(E_n) \\ \Sigma_{\downarrow\uparrow}^{GW}(E_n) & h^0 + \Sigma_{\downarrow\downarrow}^{GW}(E_n) \end{pmatrix} \begin{pmatrix} \psi_{n\uparrow} \\ \psi_{n\downarrow} \end{pmatrix} = E_n \begin{pmatrix} \psi_{n\uparrow} \\ \psi_{n\downarrow} \end{pmatrix} \quad (33)$$

which contains the effects of the non-diagonal spin components of the self-energy.

A non-interacting Green's function constructed from a Hamiltonian containing a spin-orbit interaction will also have non-diagonal spin components. A similar formulation as above can be applied to this situation. The screened interaction will contain charge-spin coupling components and the self-energy will take a more general form as given in (10). Correlation effects on orbital moments and spin densities can then be accessed including life-time effects.

In conclusion, we have derived the spin-dependent generalization of the original set of Hedin's equations. Their first order term (in the spin-dependent screened interaction) leads to a spin-dependent GW approximation. These equations allow for a truly first-principles study

of a wide range of problems where correlation effects induced by spin interactions play a crucial role in determining physical properties. Applications to nanoscale magnetic systems ranging from quantum dots, quantum wires to impurities or nanoparticles, as well as to films, surface and interface problems now come into reach [9, 10]. Also, developments at the interface of many-body perturbation theory and time-dependent density functional theory as proposed in [11, 12] are readily generalized e.g. to relativistic interactions. The same is true for combined GW and dynamical mean field techniques [13].

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